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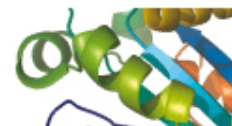
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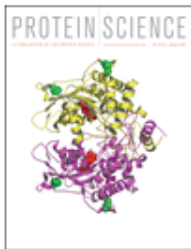
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A synergistic approach to protein crystallization: Combination of a fixed-arm carrier with surface entropy reduction (pages 901–913)
 Andrea F. Moon, Geoffrey A. Mueller, Xuejun Zhong and Lars C. Pedersen
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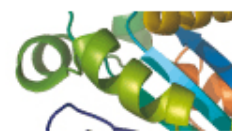
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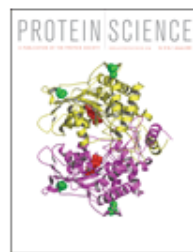
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Z. Nevin Gerek^{1,2}, S. Banu Ozkan^{1,2*}

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protein flexibility; PDZ domain; docking; selectivity; ROSETTALIGAND

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Modeling of protein binding site flexibility in molecular docking is still a challenging problem due to the large conformational space that needs sampling. Here, we propose a flexible receptor docking scheme: A dihedral restrained replica exchange molecular dynamics (REMD), where we incorporate the normal modes obtained by the Elastic Network Model (ENM) as dihedral restraints to speed up the search towards correct binding site conformations. To our knowledge, this is the first approach that uses ENM modes to bias REMD simulations towards binding induced fluctuations in docking studies. In our docking scheme, we first obtain the deformed structures of the unbound protein as initial conformations by moving along the binding fluctuation mode, and perform REMD using the ENM modes as dihedral restraints. Then, we generate an ensemble of multiple receptor conformations (MRCs) by clustering the lowest replica trajectory. Using ROSETTALIGAND, we dock ligands to the clustered conformations to predict the binding pose and affinity. We apply this method to postsynaptic density-95/Dlg/ZO-1 (PDZ) domains; whose dynamics govern their binding specificity. Our approach produces the lowest energy bound complexes with an average ligand root mean square deviation of 0.36 Å. We further test our method on (i) homologs and (ii) mutant structures of PDZ where mutations alter the binding selectivity. In both cases, our approach succeeds to predict the correct pose and the affinity of binding peptides. Overall, with this approach, we generate an ensemble of MRCs that leads to predict the binding poses and specificities of a protein complex accurately.

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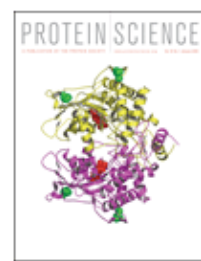
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smart sampling strategies. Recently, Abagyan and collaborators²⁹ were able to incorporate the multiple receptor conformational ensemble in a single docking simulation and reduce the sampling time with their approach.

In this present study, we come up with a novel sampling strategy by combining the ENM with replica exchange molecular dynamics (REMD)³⁰ to generate “binding induced” MRCs. Clustering molecular dynamics snapshots^{8–13} and generating conformations by perturbing the conformation along normal modes^{18, 19, 24, 31–33} have been separately applied to incorporate the receptor flexibility in

A flexible docking scheme to explore the binding selectivity of PDZ domains

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Received 20 August 2009; Revised 16 December 2009; Accepted 8 February 2010

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Published online 1 March 2010 proteinscience.org

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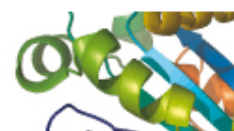
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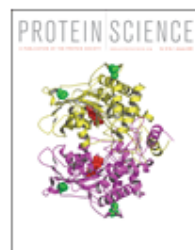
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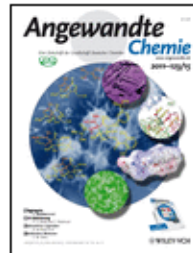
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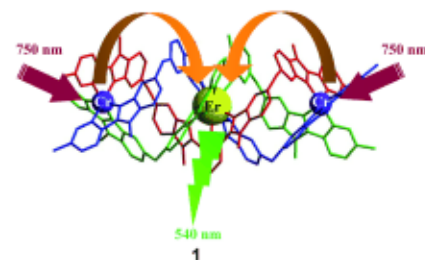
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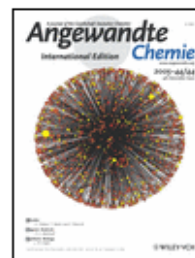
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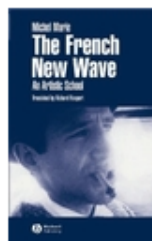
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Chapter Two

A Critical Concept

A Critical School

THE NEW WAVE DIRECTORS initially and repeatedly denied that they formed a unified movement. For instance, François Truffaut proclaimed: “I see only one common point shared by young directors: we all play pinball while older directors drink scotch and play cards.”¹ Despite the many denials, however, this artistic trend was closely tied to a collection of critical concepts held by a fairly coherent group. One of the first criteria for belonging to the New Wave was to have experience as a film critic. These young directors were all *cinéphiles*, or very devoted film buffs, who knew their film history inside out. They acquired their understanding of cinematic culture from watching thousands of films. gaining clear ideas about *mise-*

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Abscisic acid (ABA; Figure 1) is a 15-carbon sesquiterpene phytohormone found in all higher plants and in certain algae, fungi and bryophytes (Hartung and Gimmler, 1994). It has mostly been studied in higher plants and is present in all tissues. There are two enantiomeric forms of ABA (S-(+)-ABA and R-(-)-ABA) of which only (+)-ABA occurs naturally. Until recently, (+)-ABA was considered the only naturally occurring substance with ABA-like hormonal activity. However, recent studies have shown that the three hydroxylated metabolites of (+)-ABA (7'-, 8'- and 9'-hydroxyABA; Figure 2) also induce ABA-like bioactivity and may therefore contribute to the overall hormonal effects previously attributed solely to ABA itself (Zaharia *et al.*, 2005).



Figure 1. Biosynthesis of ABA from epoxycarotenoids. Dotted lines indicate possible alternate pathways. NCED; 9-*cis*-epoxycarotenoid dioxygenase.

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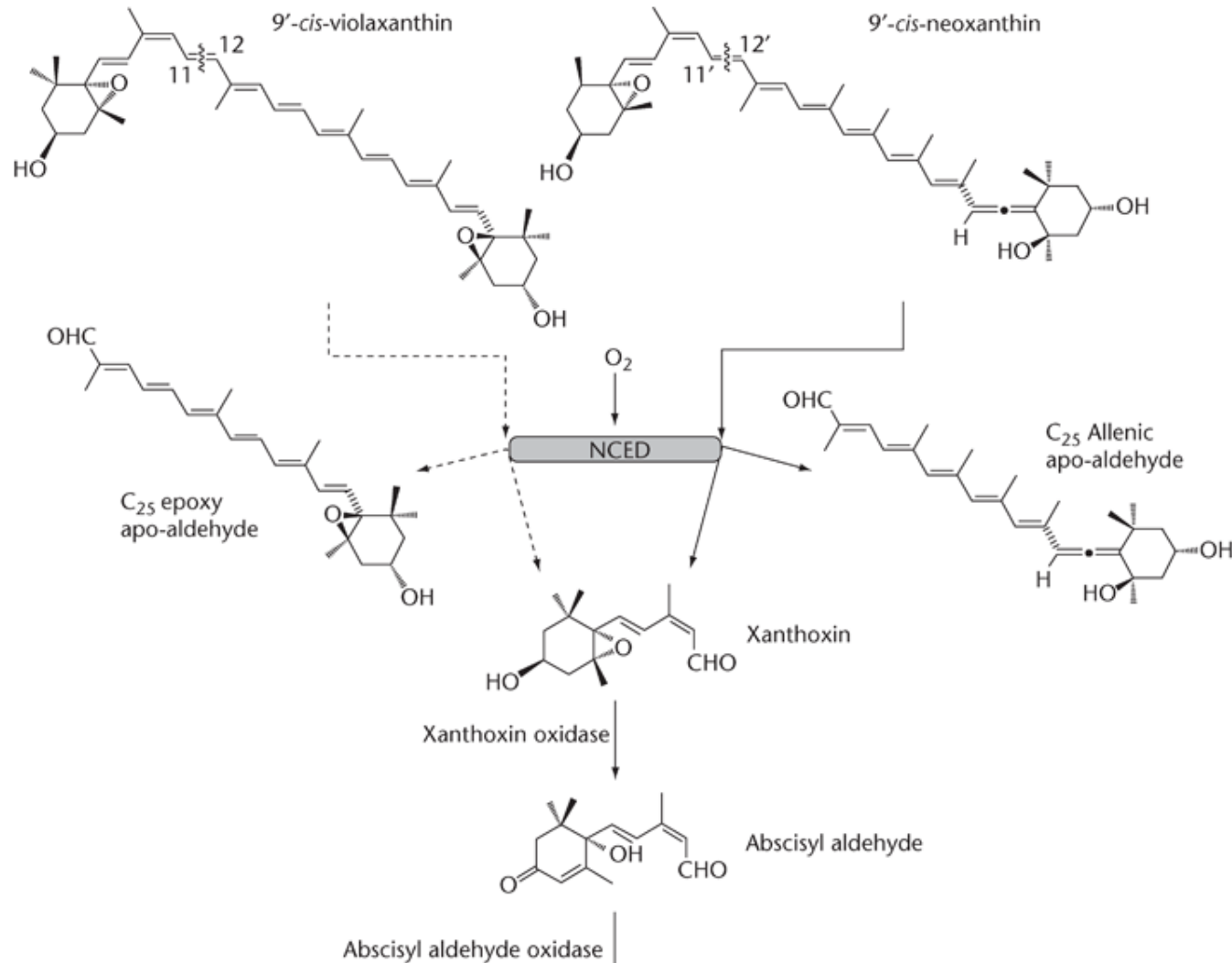
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adapt to poor growth conditions. Plants continually sense their environment and with the onset of potentially harmful changes such as reduced soil-water content or low temperature, abscisic acid levels increase throughout the plant to co-ordinate responses in all tissues. These responses are adaptive and provide a means by which a period of modest stress allows the plant to be more resistant to a subsequent period of more severe stress. This is known as acclimation. See also



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Malaria remains a major cause of illness and death in Africa and other endemic, and often resource-limited, settings. Most cases of malaria are uncomplicated but can quickly turn into severe, often fatal, episodes in vulnerable individuals if not promptly diagnosed and effectively treated. Parasitological diagnosis of malaria has for a long time been based on microscopic detection of asexual malaria parasites on a blood smear from a person suspected to have malaria. But many areas lack laboratory support...

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Anticonvulsants for tinnitus

Carlijn EL Hoekstra^{1*}, Sybren P Rynja¹,
Gijsbert A van Zanten¹, Maroeska M Rovers²

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Plain language summary

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Anticonvulsants for tinnitus

Tinnitus is the perception of sound or noise in the absence of external acoustic stimulation. It is a common and potentially distressing symptom for which no adequate therapy exists. The pathophysiology of tinnitus has been compared to phantom limb pain therefore anticonvulsant drugs have been proposed as a possible therapy.

This review includes seven studies (six low-quality and one high-quality) of four different anticonvulsants (gabapentin, carbamazepine, flunarizine and lamotrigine). We found that anticonvulsants do not have a beneficial effect in the treatment of tinnitus. Side effects of the anticonvulsants used were experienced by 18% of patients.

Background

Tinnitus is the perception of sound or noise in the absence of an external or internal acoustic stimulation. It is a common and potentially distressing symptom for which no adequate therapy exists.

Objectives

To assess the effectiveness of anticonvulsants in patients with chronic tinnitus.

Search strategy

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Hoekstra CEL, Rynja SP, van Zanten GA, Rovers MM



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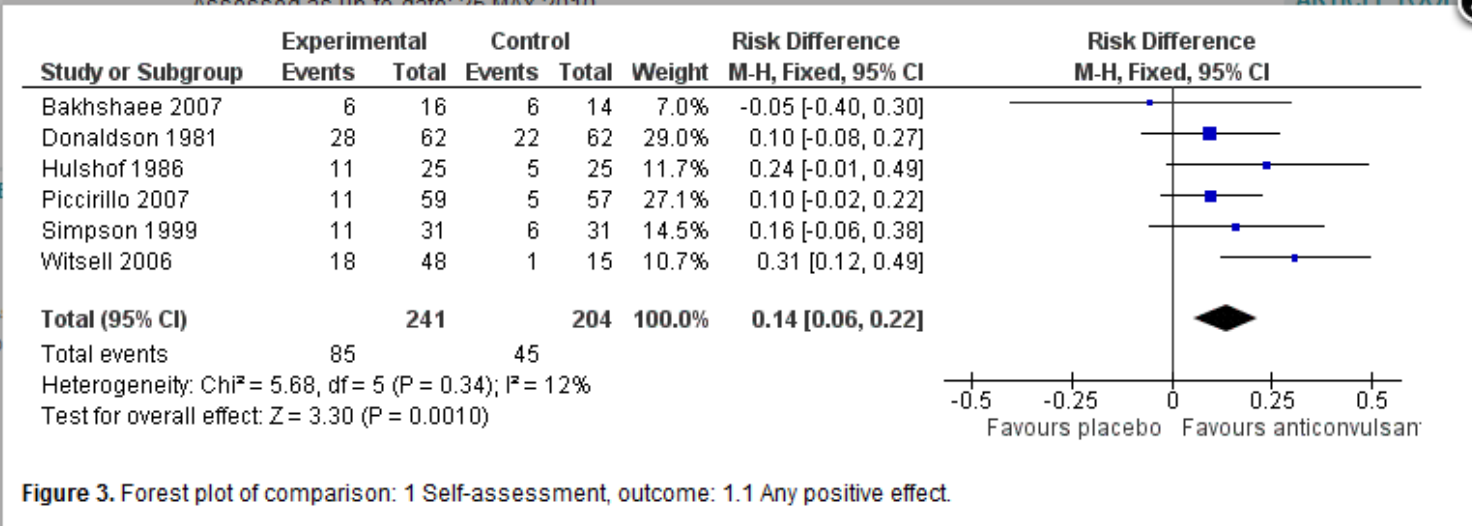


Figure 2. 'Risk of bias' summary: review authors' judgements about each methodological quality item for each included study.



Figure 3. Forest plot of comparison: 1 Self-assessment, outcome: 1.1 Any positive effect.

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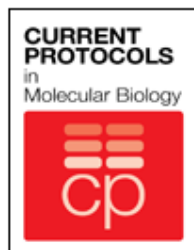
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18	10956	Acta Geologica Sinica - I	1000-9515	1755-6724	10.1111/10956	http://www	http://www	http://www	1988	1	1	1996	9	4
19	10637	Acta Medica Austriaca	0303-8173	1563-2571	10.1111/10637	http://www	http://www	http://www	2000	27	1	2003	30	2
20	9837	Acta Medica Scandinavi	0001-6101	0954-6820	10.1111/9837	http://www	http://www	http://www	1939	100	6	1939	99	2-3
21	10653	Acta Neurologica Scand	0001-6314	1600-0404	10.1111/10653	http://www	http://www	http://www	1999	100	1	1999	99	6
22	10719	Acta Neuropsychiatrica	0924-2708	1601-5215	10.1111/10719	http://www	http://www	http://www	2002	14	1	2010	22	4
23	10654	Acta Obstetricia et Gyn	0001-6349	1600-0412	10.1111/10654	http://www	http://www	http://www	1998	77	1	2005	84	12
24	10949	Acta Ophthalmologica	1755-375X	1755-3768	10.1111/10949	http://www	http://www	http://www	1923	1	1-2	1931	9	1-4
25	10655	Acta Ophthalmologica S	1395-3907	1600-0420	10.1111/10655	http://www	http://www	http://www	1995	73	1	2007	85	thesis3
26	10812	Acta Pharmacologica Sii	1671-4083	1745-7254	10.1111/10812	http://www	http://www	http://www	2005	26	1	2008	29	12

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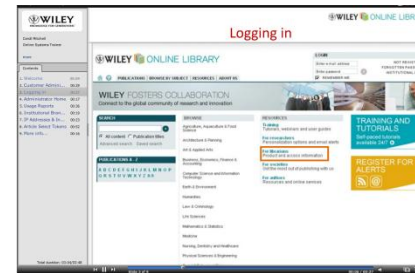
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13 Apr 2011 14:00	The Cochrane Library... PROSISE	Greta Doonan	1 hour	1 of 1
13 Apr 2011 14:30	Administration and usage of...	Nigel Thompson	40 mins	1 of 1
14 Apr 2011 14:30	Wiley Online Lib...	Nigel Thompson	40 mins	1 of 1
19 Apr 2011 15:30	The Cochrane Library... an...	Nigel Thompson	1 hour	1 of 1
20 Apr 2011 9:00	The Cochrane Library... an...	Greta Doonan	1 hour	1 of 1
23 Apr 2011 14:30	Online Books and Reference Ser...	Nigel Thompson	30 mins	1 of 1
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